Non-relativistic bound states in a finite volume

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Abstract

We derive general results for the mass shift of bound states with angular momentum $\ell \geq 1$ in a periodic cubic box in two and three spatial dimensions. Our results have applications to lattice simulations of hadronic molecules, halo nuclei, and Feshbach molecules. The sign of the mass shift can be related to the symmetry properties of the state under consideration. We verify our analytical results with explicit numerical calculations. Moreover, we comment on the relations connecting the effective range parameter, the binding momentum of a given state and the asymptotic normalization coefficient of the corresponding wave function. We give explicit expressions for this relation in the shallow binding limit.

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I. INTRODUCTION

Lattice simulations are used in many areas of quantum physics, ranging from nuclear and particle physics to atomic and condensed matter physics [1–3]. In such calculations the system is solved numerically using a discrete spacetime lattice over a finite volume. In practice this finite volume is usually taken to be a cubic box with periodic boundaries. When simulating composite objects such as bound states, the boundaries of the periodic box will modify quantum wave functions. This leads to finite volume shifts in the binding energies, and detailed knowledge of these finite volume effects is necessary to improve high precision lattice calculations.

In Ref. [4], Lüscher derived a formula for the finite volume mass shift of S-wave bound states of two particles with reduced mass μ interacting via a potential with finite range R. When a bound state with energy $-E_B$ is put in a periodic cubic box of length L, its energy in the rest frame is shifted by an amount

$$\Delta m_B = -3|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,, \tag{1}$$

where $\kappa = \sqrt{2\mu E_B}$ is the binding momentum and γ is the asymptotic wave function normalization defined by $\psi_B(r) = \gamma\,\mathrm{e}^{-\kappa r}/(\sqrt{4\pi}r)$ for $r > R$. For potentials with exponential fall-off, $V(r) \sim \exp(-r/R)$ for large r, the formula is modified by exponentially small corrections when the binding momentum κ is smaller than $1/R$. Bound states moving in a finite periodic volume also have a topological phase correction to the energy [5, 6]. This topological phase correction contains information about the number and mass of the constituents of the bound states. It must be included when determining scattering phase shifts for composite objects in a finite volume.

In Ref. [7], we briefly discussed the generalization of Lüscher's formula (1) for the finite volume mass shift to higher partial waves. In this paper, we present the full derivation of these results. Moreover, we give the general mass shift for states with angular momenta up to $\ell = 3$. In general, the mass shift for a given state depends on its transformation properties with respect to the symmetry group of the cubic box. In addition to reducing finite volume effects from precision lattice calculations, our finite volume results can also be used as a diagnostic tool to probe the angular momentum and radial structure of the bound state wave function. A summary of our results is given by Eq. (66) together with Table I at the end of Sec. IV A. We also derive a general mass shift formula for two-dimensional systems in a finite area with periodic boundaries.

In our discussion here we only consider stable bound states. However, resonances above continuum thresholds can also be described from the volume dependence of avoided level crossings [8, 9]. Our results are universal and can be applied to a wide range of systems. We will discuss a few examples below.

In particle physics, there is some interest in hadronic molecules with angular momentum [10–12]. In the case of S-waves, the deuteron and some exotic weakly bound states such as the H-dibaryon were recently studied in lattice QCD [13]. Similar investigations for exotic bound states with angular momentum appear feasible in the future. In atomic physics, several experiments have investigated strongly-interacting P-wave Feshbach resonances in ^{6}Li and ^{40}K [14–16], which can be tuned to produce bound P-wave dimers. If such systems are simulated in a finite volume, our results can be used to describe the finite volume dependence of the dimers.

Halo nuclei constitute a special class of weakly-bound nuclei with molecular character. They consist of a compact core and one or more nucleons with low separation energy [17]. Among halo nuclei there are some systems with nonzero orbital angular momentum. A well-known example of a P-wave halo state is the $J^P = 1/2^-$ excited state in ^{11}Be. The electromagnetic properties of the low-lying states in this nucleus can be well described in a two-body halo picture of a ^{10}Be core and a neutron [18, 19]. A similar strategy was applied to radiative neutron capture on ^{7}Li [20]. A related class of systems is given by nuclei with an α-cluster structure such as ^{8}Be and excited states of ^{12}C [21–23]. The Hoyle state in ^{12}C was recently calculated for the first time in an *ab initio* approach using chiral effective field theory and nuclear lattice calculations [23]. Understanding the finite volume corrections is crucial in such a calculation. Due to the α-cluster structure, the volume dependence of the Hoyle state is governed by the volume dependence of a three-body system. Finally, we note that the asymptotic normalization coefficient of the bound state wave function appears in the mass shift formula. Hence, our results can be used to extract this quantity from lattice calculations at finite volume. The asymptotic normalization is directly connected to zero-energy capture reactions [24], which play an important role in nuclear astrophysics.

The paper is organized as follows. We start with some prerequisites and a general discussion of the finite volume mass shift in Section II. Lüscher's result for S-waves is reviewed in Section III, while our extension to higher partial waves is given in Section IV. In particular, we discuss the mass shift for the irreducible representations of the cubic group, relate the sign of the shift to the leading parity, and derive a trace formula for the multiplet-averaged mass shift for states with arbitrary angular momentum ℓ. In Section V, we verify our results numerically for two model systems. The case of two spatial dimensions is treated in Section VI. Finally, a brief summary and outlook is given in Section VII. In the appendix, we discuss the relation of the asymptotic normalization constant to scattering parameters and derive explicit shallow binding relations between the effective range, the binding momentum and the asymptotic normalization coefficient.

II. BOUND STATES IN A FINITE VOLUME

As a starting point, we first review several results from [4]. We closely follow Lüscher's derivation, but consider a more general system with arbitrary angular momentum and non-local interactions.

A. Definitions and basic identities

We start with some definitions and basic identities about bound states in rotationally symmetric potentials $V(r)$. This will also help to define our notation used throughout the discussion. For a bound state with energy $E = -E_B$ and angular-momentum quantum numbers (ℓ, m), we separate the wave function $\psi(\mathbf{r})$ as a product of the radial wave function $u_\ell(r)$ and spherical harmonics $Y_\ell^m(\theta, \phi)$,

$$\psi(\mathbf{r}) = R_\ell(r) Y_\ell^m(\theta, \phi) = \frac{u_\ell(r)}{r} Y_\ell^m(\theta, \phi)\,. \tag{2}$$

This leads to the radial Schrödinger equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\ell(\ell+1)}{r^2} - U(r) + p^2\right] u_\ell(r) = 0\,, \tag{3}$$

with $p = \sqrt{2\mu E} = \sqrt{-2\mu E_B} \equiv \mathrm{i}\kappa$ and $U(r) \equiv 2\mu V(r)$. The mass is denoted by μ since in later applications it will be the reduced mass for a two-particle system. The normalized radial wave function satisfies

$$\int_0^\infty \mathrm{d}r\, |u_\ell(r)|^2 = 1\,. \tag{4}$$

For vanishing potential, we have two linearly independent solutions of the free wave equation. These are the Riccati–Bessel functions $\hat{\jmath}_\ell(pr)$ and Riccati–Neumann functions $\hat{n}_\ell(pr)$, which can be expressed in terms of ordinary Bessel functions. It is often more convenient to work with the Riccati–Hankel functions

$$\hat{h}^\pm_\ell(z) = \hat{n}_\ell(z) \pm \mathrm{i}\hat{\jmath}_\ell(z). \tag{5}$$

These have the asymptotic form $\mathrm{e}^{\pm\mathrm{i}z}$ as $|z| \to \infty$. For future reference, we give the explicit expressions for $\hat{h}^+_\ell(z)$ for $\ell = 0, 1, 2$:

$$\hat{h}^+_0(z) = \mathrm{e}^{\mathrm{i}z}\,, \tag{6a}$$

$$\hat{h}^+_1(z) = \left(1 + \frac{\mathrm{i}}{z}\right) \mathrm{e}^{\mathrm{i}(z-\pi/2)}\,, \tag{6b}$$

$$\hat{h}^+_2(z) = \left(1 + \frac{3\mathrm{i}}{z} - \frac{3}{z^2}\right) \mathrm{e}^{\mathrm{i}(z-\pi)}\,. \tag{6c}$$

Asymptotic form of bound state wave functions

In order to discuss the asymptotic form of bound state wave functions we define solutions $\chi^\pm_{\ell,p}(r)$ of (3) that fulfill the condition

$$\chi^\pm_{\ell,p}(r) \xrightarrow{r\to\infty} \hat{h}^\pm_\ell(pr)\,. \tag{7}$$

The bound-state solution normalized according to (4) can then be written as

$$u_\ell(r) = \mathrm{i}^\ell \gamma\, \chi^+_{\ell,p}(r)\,, \tag{8}$$

where $p = \mathrm{i}\kappa$ and

$$\gamma = \left(\int_0^\infty \mathrm{d}r\, |\chi^+_{\ell,p}(r)|^2\right)^{-1/2} \tag{9}$$

is the asymptotic normalization coefficient.[1] The factor i^ℓ adjusts the phase such that $u_\ell(r)$ is a real function. If the potential has a finite range R, *i.e.*, $U(r) = 0$ for $r > R$, we have the exact identity

$$u_\ell(r) = \mathrm{i}^\ell \gamma\, \hat{h}^+_\ell(\mathrm{i}\kappa r) \quad \text{for} \quad r > R\,. \tag{10}$$

[1] For more details, see Ref. [25], Chaps. 11 and 12.

The asymptotic normalization γ is itself an interesting quantity. In low-energy astrophysical reactions it determines the capture rate of a single proton or neutron at zero relative energy [24]. In the shallow binding limit it is also directly related to low-energy scattering parameters. For $\ell = 0$,

$$r_0 + \frac{2}{\gamma^2} - \frac{1}{\kappa} = \mathcal{O}(\kappa) \quad \text{as} \quad \kappa \to 0\,, \tag{11a}$$

whereas for angular momenta $\ell \geq 1$ one has

$$r_\ell + \frac{2\kappa^{2\ell}}{\gamma^2} = \mathcal{O}(\kappa) \quad \text{as} \quad \kappa \to 0\,. \tag{11b}$$

We note that γ will in general depend upon the binding momentum κ. We will derive the relations (11a) and (11b) in Appendix A. The S-wave formula is well known and given in [26], although without the $\mathcal{O}(\kappa)$ correction estimate. For higher angular momentum the situation is qualitatively different due to the divergence of $\hat{h}_\ell^+(z)$ at $z = 0$.

B. Infinite volume

We now consider a system of two spinless particles with reduced mass μ with zero total momentum. We will work with relative coordinates $\mathbf{r} = \vec{r}_1 - \vec{r}_2$. The interaction is given by a potential $V(\mathbf{r}, \mathbf{r}')$, which we in general allow to be non-local in configuration space. It is assumed to be Hermitian, rotationally symmetric, and to have a finite range R, *i.e.*,

$$V(\mathbf{r}, \mathbf{r}') = 0 \quad \text{if} \quad |\mathbf{r}| > R \quad \text{or} \quad |\mathbf{r}'| > R\,. \tag{12}$$

We consider the case when the system has a bound state $|\psi_B\rangle$ with angular quantum numbers (ℓ, m). The Schrödinger equation,

$$\hat{H}\,|\psi_B\rangle = -E_B\,|\psi_B\rangle\ , \tag{13}$$

can be written as

$$-\frac{1}{2\mu}\Delta_r\,\psi_B(\mathbf{r}) + \int \mathrm{d}^3r'\,V(\mathbf{r}, \mathbf{r}')\,\psi_B(\mathbf{r}') = -E_B\,\psi_B(\mathbf{r}) \tag{14}$$

in configuration space. We note that for a local potential,

$$V(\mathbf{r}, \mathbf{r}') = V(\mathbf{r})\,\delta^{(3)}(\mathbf{r} - \mathbf{r}')\,, \tag{15}$$

Eq. (14) reduces to the familiar form

$$\left[-\frac{1}{2\mu}\Delta_r\ + V(\mathbf{r})\right]\,\psi_B(\mathbf{r}) = -E_B\,\psi_B(\mathbf{r})\,. \tag{16}$$

Regardless of the locality of the interaction, the wave function $\psi_B(\mathbf{r})$ has the asymptotic form

$$\psi_B(\mathbf{r}) = \mathrm{i}^\ell \gamma\, Y_\ell^m(\mathbf{r}/r)\,\frac{\hat{h}_\ell^+(i\kappa r)}{r} \quad (r > R)\,, \tag{17}$$

where $\kappa = \sqrt{2\mu E_B}$ is the binding momentum.

C. Finite volume

We now consider what happens when the two-body system is put into a cubic periodic box with length $L \gg R$. For this problem it is convenient to define a periodic extension of the potential

$$V_L(\mathbf{r}, \mathbf{r}') = \sum_{\mathbf{n} \in \mathbb{Z}^3} V(\mathbf{r} + \mathbf{n}L, \mathbf{r}' + \mathbf{n}L) \,. \tag{18}$$

We take $|\psi\rangle$ to be an exact periodic solution of the finite volume Schrödinger equation,

$$\hat{H}_L \, |\psi\rangle = -E_B(L) \, |\psi\rangle \ , \tag{19}$$

with the finite-volume Hamiltonian $\hat{H}_L = \hat{H}_0 + \hat{V}_L$. It is clear that $E_B(L)$ approaches the infinite volume eigenvalue E_B and $|\psi\rangle \to |\psi_B\rangle$ as $L \to \infty$.

We now derive a formula for the finite volume mass (energy) shift,

$$\Delta m_B \equiv E_B(\infty) - E_B(L) \,. \tag{20}$$

Let us define a state $|\psi_0\rangle$ by adding together periodic copies of the infinite volume wave function in (14),

$$\langle \mathbf{r} | \psi_0 \rangle = \psi_0(\mathbf{r}) = \sum_{\mathbf{n}} \psi_B(\mathbf{r} + \mathbf{n}L) \,. \tag{21}$$

This clearly satisfies the periodicity condition. Acting upon this state with the finite volume Hamiltonian, we get

$$\begin{aligned} H_L \psi_0(\mathbf{r}) &= H_0 \sum_{\mathbf{n}'} \psi_B(\mathbf{r} + \mathbf{n}'L) + \sum_{\mathbf{n}'} \sum_{\mathbf{n}} \int \mathrm{d}^3 r' \, V(\mathbf{r} + \mathbf{n}L, \mathbf{r}' + \mathbf{n}L) \psi_B(\mathbf{r}' + \mathbf{n}'L) \\ &= \sum_{\mathbf{n}'} \Bigg\{ H_0 \, \psi_B(\mathbf{r} + \mathbf{n}'L) + \int \mathrm{d}^3 r' \, V(\mathbf{r} + \mathbf{n}'L, \mathbf{r}' + \mathbf{n}'L) \, \psi_B(\mathbf{r}' + \mathbf{n}'L) \\ &\qquad\qquad + \sum_{\mathbf{n} \neq \mathbf{n}'} \int \mathrm{d}^3 r' \, V(\mathbf{r} + \mathbf{n}L, \mathbf{r}' + \mathbf{n}L) \, \psi_B(\mathbf{r}' + \mathbf{n}'L) \Bigg\} \\ &= -E_B(\infty) \sum_{\mathbf{n}'} \psi_B(\mathbf{r} + \mathbf{n}'L) + \sum_{\mathbf{n}'} \sum_{\mathbf{n} \neq \mathbf{n}'} \int \mathrm{d}^3 r' \, V(\mathbf{r} + \mathbf{n}L, \mathbf{r}' + \mathbf{n}L) \, \psi_B(\mathbf{r} + \mathbf{n}'L) \,. \end{aligned} \tag{22}$$

The final result can be written as

$$\hat{H}_L \, |\psi_0\rangle = -E_B(\infty) \, |\psi_0\rangle + |\eta\rangle \ , \tag{23}$$

where we have defined $|\eta\rangle$ as

$$\eta(\mathbf{r}) = \sum_{\mathbf{n}'} \sum_{\mathbf{n} \neq \mathbf{n}'} \int \mathrm{d}^3 r' \, V(\mathbf{r} + \mathbf{n}L, \mathbf{r}' + \mathbf{n}L) \, \psi_B(\mathbf{r}' + \mathbf{n}'L) \,. \tag{24}$$

With the substitution $\mathbf{r}' \to \mathbf{r}' - \mathbf{n}L$ for each term in the sum, this can be rewritten as

$$\eta(\mathbf{r}) = \sum_{\mathbf{n}'} \sum_{\mathbf{n} \neq \mathbf{n}'} \int \mathrm{d}^3 r' \, V(\mathbf{r} + \mathbf{n}L, \mathbf{r}') \, \psi_B\big(\mathbf{r}' + (\mathbf{n}' - \mathbf{n})L\big) \,. \tag{25}$$

Due to the finite range of the potential we only get contributions from the domain $|\mathbf{r}'| < R$. We note that $|\mathbf{r}' + (\mathbf{n}' - \mathbf{n})L| > R$ when $\mathbf{n} \neq \mathbf{n}'$ and $R \ll L$. Therefore we can use the asymptotic form of the wave function and find that $|\eta\rangle = \mathcal{O}\big(\mathrm{e}^{-\kappa L}\big)$. This means that $|\psi_0\rangle$ is an approximate solution of the finite volume Schrödinger equation (19) for large L. Motivated by this, we write the exact finite volume solution $|\psi\rangle$ explicitly as

$$|\psi\rangle = \alpha\,|\psi_0\rangle + |\psi'\rangle \quad \text{with} \quad |\psi'\rangle = \mathcal{O}\big(\mathrm{e}^{-\kappa L}\big)\,. \tag{26}$$

We take $|\psi\rangle$ to be unit-normalized per volume L^3. The same is true of $|\psi_0\rangle$ up to corrections of order $\mathrm{e}^{-\kappa L}$. We will choose α such that

$$\langle\psi'|\psi_0\rangle = 0\,. \tag{27}$$

Consider now the matrix element $\langle\psi|\,\hat{H}_L\,|\psi_0\rangle$. Acting with $\hat{H}_L$ on $|\psi_0\rangle$, we get

$$\langle\psi|\,\hat{H}_L\,|\psi_0\rangle = -E_B(\infty)\,\langle\psi|\psi_0\rangle + \langle\psi|\eta\rangle = -E_B(\infty)\,\langle\psi_0|\psi_0\rangle\cdot\alpha + \langle\psi|\eta\rangle \tag{28}$$

according to (23) and (26). On the other hand, acting with $\hat{H}_L$ on $\langle\psi|$ yields

$$\langle\psi|\,\hat{H}_L\,|\psi_0\rangle = -E_B(L)\,\langle\psi|\psi_0\rangle = -E_B(L)\,\langle\psi_0|\psi_0\rangle\cdot\alpha\,. \tag{29}$$

Combining these two results we find

$$E_B(\infty) - E_B(L) = \Delta m_B = \frac{\langle\psi|\eta\rangle}{\alpha\,\langle\psi_0|\psi_0\rangle}\,. \tag{30}$$

We first consider the numerator in this expression. Obviously,

$$\langle\psi|\eta\rangle = \alpha\,\langle\psi_0|\eta\rangle + \langle\psi'|\eta\rangle = \alpha\,\langle\psi_0|\eta\rangle + \mathcal{O}\big(\mathrm{e}^{-2\kappa L}\big)\,. \tag{31}$$

We note that the factor of α here will cancel the α in the denominator of (30). We can now simplify further starting with

$$\langle\psi_0|\eta\rangle = \sum_{\mathbf{n}''}\sum_{\mathbf{n}'}\sum_{\mathbf{n}\neq\mathbf{n}'}\int \mathrm{d}^3r\int \mathrm{d}^3r'\,\psi_B^*(\mathbf{r}+\mathbf{n}''L)\,V(\mathbf{r}+\mathbf{n}L,\mathbf{r}'+\mathbf{n}L)\,\psi_B(\mathbf{r}'+\mathbf{n}'L)\,. \tag{32}$$

For each $\mathbf{n}$ we can make the substitutions $\mathbf{r}\to\mathbf{r}-\mathbf{n}L$ and $\mathbf{r}'\to\mathbf{r}'-\mathbf{n}L$. These leave the integrals invariant, and we get

$$\langle\psi_0|\eta\rangle = \sum_{\mathbf{n}''}\sum_{\mathbf{n}'}\sum_{\mathbf{n}\neq\mathbf{n}'}\int \mathrm{d}^3r\int \mathrm{d}^3r'\,\psi_B^*\big(\mathbf{r}+(\mathbf{n}''-\mathbf{n})L\big)\,V(\mathbf{r},\mathbf{r}')\,\psi_B\big(\mathbf{r}'+(\mathbf{n}'-\mathbf{n})L\big)\,. \tag{33}$$

Setting $\mathbf{m}=\mathbf{n}'-\mathbf{n}$ and $\mathbf{m}'=\mathbf{n}''-\mathbf{n}$ yields

$$\langle\psi_0|\eta\rangle = C\cdot\sum_{\mathbf{m}'}\sum_{\mathbf{m}\neq\mathbf{0}}\int \mathrm{d}^3r\int \mathrm{d}^3r'\,\psi_B^*(\mathbf{r}+\mathbf{m}'L)\,V(\mathbf{r},\mathbf{r}')\,\psi_B(\mathbf{r}'+\mathbf{m}L)\,, \tag{34}$$

where C counts the number of repeated periodic copies. The fact that C diverges simply reflects the fact that we are working with periodic wave functions with normalization measured per volume L^3, and C will cancel in the final result. For the integral to be non-zero,

both $\mathbf{r}$ and $\mathbf{r}'$ have to be close to $\mathbf{0}$ due to the finite range of the potential. From the assumption $L \gg R$ it then follows that all terms with $\mathbf{m}' \neq \mathbf{0}$ are suppressed by at least a factor of $\mathrm{e}^{-2\kappa L}$, and we have

$$\langle\psi_0|\eta\rangle = C \cdot \sum_{\mathbf{m}\neq\mathbf{0}} \int \mathrm{d}^3r \int \mathrm{d}^3r'\, \psi_B^*(\mathbf{r})\, V(\mathbf{r},\mathbf{r}')\, \psi_B(\mathbf{r}'+\mathbf{m}L) + \mathcal{O}\big(\mathrm{e}^{-2\kappa L}\big)\,. \tag{35}$$

The possible nonvanishing values of $|\mathbf{m}|$ are $1, \sqrt{2}, \sqrt{3}, \ldots$. We therefore arrive at

$$\langle\psi_0|\eta\rangle = C \cdot \sum_{|\mathbf{m}|=1} \int \mathrm{d}^3r \int \mathrm{d}^3r'\, \psi_B^*(\mathbf{r})\, V(\mathbf{r},\mathbf{r}')\, \psi_B(\mathbf{r}'+\mathbf{m}L) + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{36}$$

For the denominator in (30), an analogous procedure yields

$$\langle\psi_0|\psi_0\rangle = C \cdot \sum_{\mathbf{m}} \int \mathrm{d}^3r\, \psi_B^*(\mathbf{r})\, \psi_B(\mathbf{r}+\mathbf{m}L) = C \cdot \big[1 + \mathcal{O}\big(\mathrm{e}^{-\kappa L}\big)\big] \tag{37}$$

with the same constant C as above. Combining (36) and (37), the constant C cancels and we get

$$\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3r \int \mathrm{d}^3r'\, \psi_B^*(\mathbf{r})\, V(\mathbf{r},\mathbf{r}')\, \psi_B(\mathbf{r}'+\mathbf{n}L) + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,, \tag{38}$$

where we have renamed $\mathbf{m}$ back to $\mathbf{n}$.

Eq. (38) is a general result valid for any angular momentum. The dependence of the mass shift upon quantum numbers (ℓ, m) will emerge from the wave function ψ_B and the resulting overlap integrals in (38). In the following, we explore this dependence in detail and denote the mass shift as $\Delta m_B^{(\ell,m)}$.

III. LÜSCHER'S RESULT FOR S-WAVES

For $\ell = 0$ the asymptotic wave function (17) is given as

$$\psi_B(\mathbf{r}) = \psi_B(|\mathbf{r}|) = \sqrt{\frac{1}{4\pi}}\,\frac{u_0(r)}{r} \tag{39a}$$

with

$$u_0(r) = \gamma\, \hat{h}_0^+(\mathrm{i}\kappa r) = \gamma\, \mathrm{e}^{-\kappa r} \quad \text{for} \quad r > R\,. \tag{39b}$$

Due to the finite range $R \ll L$ of the potential we only have contributions with $|\mathbf{r}'+\mathbf{n}L| > R$ in (38). Hence we can insert the asymptotic form for $\psi_B(\mathbf{r}'+\mathbf{n}L)$ and get

$$\Delta m_B^{(0,0)} = \frac{\gamma}{\sqrt{4\pi}} \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3r \int \mathrm{d}^3r'\, \psi_B^*\big(|\mathbf{r}|\big)\, V(\mathbf{r},\mathbf{r}')\, \frac{\mathrm{e}^{-\kappa|\mathbf{r}'+\mathbf{n}L|}}{|\mathbf{r}'+\mathbf{n}L|} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{40}$$

We can furthermore use the Schrödinger equation (14) to eliminate the potential. Doing this and then renaming $\mathbf{r}' \to \mathbf{r}$, we get

$$\begin{aligned} \Delta m_B^{(0,0)} &= \frac{\gamma}{\sqrt{4\pi}} \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3r \left\{ \left[\frac{\Delta_r}{2\mu} - E_B\right] \psi_B^*\big(|\mathbf{r}|\big) \right\} \frac{\mathrm{e}^{-\kappa|\mathbf{r}+\mathbf{n}L|}}{|\mathbf{r}+\mathbf{n}L|} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big) \\ &= \frac{\gamma}{\sqrt{4\pi}} \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3r\, \psi_B^*\big(|\mathbf{r}-\mathbf{n}L|\big) \frac{1}{2\mu} \left[\Delta_r - \kappa^2\right] \frac{\mathrm{e}^{-\kappa r}}{r} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \end{aligned} \tag{41}$$

In the second line we have shifted the integration variable and used partial integration to let the Laplacian act on $\exp(-\kappa r)/r$. Finally, we use the fact that $\exp(-\kappa r)/(4\pi r)$ is a Green's function for the operator $\Delta_r - \kappa^2$,

$$\left[\Delta_r - \kappa^2\right] \frac{\mathrm{e}^{-\kappa r}}{4\pi r} = -\delta^{(3)}(\mathbf{r})\,. \tag{42}$$

This allows us to perform the integral and arrive at

$$\begin{aligned} \Delta m_B^{(0,0)} &= -\frac{\sqrt{\pi}\gamma}{\mu} \sum_{|\mathbf{n}|=1} \psi_B^*\big(|\mathbf{n}L|\big) + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big) \\ &= -3|\gamma|^2\, \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big). \end{aligned} \tag{43}$$

In the last step we have inserted the asymptotic form of the wave function for $\psi_B^*\big(|\mathbf{n}L|\big) = \psi_B^*(L)$, and the sum yields a factor of six. This is just Lüscher's result (1) as given in the introduction.

IV. EXTENSION TO HIGHER PARTIAL WAVES

We now discuss the generalization of the mass shift formula to arbitrary angular momentum. The general form for the asymptotic wave function is

$$\psi_{B,(\ell,m)}(\mathbf{r}) = Y_\ell^m(\theta,\phi)\, \frac{\mathrm{i}^\ell \gamma \hat{h}_\ell^+(\mathrm{i}\kappa r)}{r}\,. \tag{44}$$

Inserting this into (38) and performing steps analogous to those presented above for the S-wave case, we find

$$\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r\, \left\{ \frac{1}{2\mu}\big[\Delta_r - \kappa^2\big] \psi_B^*(\mathbf{r} - \mathbf{n}L) \right\} Y_\ell^m(\theta,\phi) \frac{\mathrm{i}^\ell \gamma \hat{h}_\ell^+(\mathrm{i}\kappa r)}{r} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{45}$$

The crucial ingredient is the relation

$$Y_\ell^m(\theta,\phi)\, \frac{\hat{h}_\ell^+(\mathrm{i}\kappa r)}{r} = (-\mathrm{i})^\ell\, R_\ell^m\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r\right)\left[\frac{\mathrm{e}^{-\kappa r}}{r}\right], \tag{46}$$

where R_ℓ^m are the solid harmonics defined via $R_\ell^m(x,y,z) = R_\ell^m(\mathbf{r}) = r^\ell Y_\ell^m(\theta,\phi)$. The derivation of (46) follows from Lemma B.1 in Ref. [28], which proves that

$$R_\ell^m(\boldsymbol{\nabla}) f(r) = R_\ell^m(\mathbf{r}) \left(\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)^\ell f(r) \tag{47}$$

for any smooth function $f(r)$. We obtain (46) by using the relation[2],

$$\left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^\ell h_0^{(1)}(z) = (-1)^\ell\, z^{-\ell}\, h_\ell^{(1)}(z)\,, \tag{48}$$

[2] The relation (48) is just a special case of Eq. (10.1.24) in [27], which also holds for other spherical Bessel functions.

and noting that $\mathrm{e}^{-\kappa r} = \hat{h}_0^+(\mathrm{i}\kappa r)$ and $\hat{h}_\ell^+(z) = \mathrm{i}z\, h_\ell^{(1)}(z)$, where $h_\ell^{(1)}(z)$ is a spherical Hankel function of the first kind.

We can illustrate (46) using an example. For the case $\ell = 1$ and $m = 0$ we have

$$\hat{h}_1^+(\mathrm{i}\kappa r) \sim \left(1 + \frac{1}{\kappa r}\right) \frac{\mathrm{e}^{-\kappa r}}{r} \tag{49}$$

and $Y_1^0(\theta, \phi) \propto \cos\theta$. A straightforward calculation shows that indeed

$$\cos\theta \left(1 + \frac{1}{\kappa r}\right) \frac{\mathrm{e}^{-\kappa r}}{r} = -\frac{1}{\kappa} \frac{\partial}{\partial z} \left[\frac{\mathrm{e}^{-\kappa r}}{r}\right], \tag{50}$$

with $\cos\theta = z/r$.

Using (46) to rewrite (45), we get

$$\Delta m_B = \frac{\gamma}{2\mu} \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r \left\{ \left[\Delta_r - \kappa^2\right] \psi_B^*(\mathbf{r} - \mathbf{n}L) \right\} \left\{ R_\ell^m \left(-\frac{1}{\kappa} \boldsymbol{\nabla}_r\right) \left[\frac{\mathrm{e}^{-\kappa r}}{r}\right] \right\} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{51}$$

We now integrate by parts and pass the Laplacian through the differential operator $R_\ell^m(-\boldsymbol{\nabla}_r/\kappa)$. Since the operators both consist of partial derivatives, this is not a problem when the wave function is smooth. We assume that this is the case, with the possible exception of a measure zero region that can be omitted from the integral.

The partial integrations give a factor $(-1)^\ell$. We can now proceed in exactly the same way as for S-waves. We perform one more integration by parts so that the Laplacian acts on $\exp(-\kappa r)/r$. This yields a delta function times a factor of -4π, and the final result is then

$$\Delta m_B^{(\ell,m)} = (-1)^{\ell+1} \cdot \frac{2\pi\gamma}{\mu} \sum_{|\mathbf{n}|=1} R_\ell^m \left(-\frac{1}{\kappa} \boldsymbol{\nabla}_r\right) \psi_{B,(\ell,m)}^*(\mathbf{r} - \mathbf{n}L) \bigg|_{\mathbf{r}=\mathbf{0}} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{52}$$

For $\psi_{B,(\ell,m)}^*$ we can insert the asymptotic form (44) since it is evaluated in the asymptotic region.

A. Results

For $\ell = 1$, we find the same result for all three P-wave states,

$$\Delta m_B^{(1,0)} = \Delta m_B^{(1,\pm 1)} = 3|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{53}$$

When compared to the S-wave case, the sign of the P-wave mass shift is reversed while the magnitude is the same. Qualitatively, this means that S-wave bound states are more deeply bound when put in a finite volume while P-wave bound states are less bound. This will be discussed in more detail later.

We next discuss the results for $\ell = 2$. From (52), we find

$$\Delta m_B^{(2,0)} = -15|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} \cdot F_2^0\big(\tfrac{1}{\kappa L}\big) + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,, \tag{54}$$

$$\Delta m_B^{(2,\pm 1)} = +15|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} \cdot F_2^1\big(\tfrac{1}{\kappa L}\big) + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,, \tag{55}$$

$$\Delta m_B^{(2,\pm 2)} = -15|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} \cdot F_2^2\big(\tfrac{1}{\kappa L}\big) + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,, \tag{56}$$

where

$$F_2^0(x) = \frac{1}{2} + 3x + \frac{27}{2}x^2 + \frac{63}{2}x^3 + \frac{63}{2}x^4\,, \tag{57}$$

$$F_2^1(x) = 2x + 9x^2 + 21x^3 + 21x^4\,, \tag{58}$$

$$F_2^2(x) = \frac{1}{4} + \frac{1}{2}x + \frac{9}{4}x^2 + \frac{21}{4}x^3 + \frac{21}{4}x^4\,. \tag{59}$$

We note that the size and even the sign of the mass shift depends on the quantum number m. To understand this effect, we need to take into account that our cubic finite volume breaks the rotational symmetry group down to a cubic subgroup.

Representations of the cubic group

The cubic symmetry group $\mathcal{O}$ is a finite subgroup of $SO(3)$ with 24 elements. There are five irreducible representations of $\mathcal{O}$. They are conventionally called A_1, A_2, E, T_1 and T_2, and their dimensionalities are 1, 1, 2, 3 and 3, respectively. Irreducible representations D^ℓ of the rotation group $SO(3)$ are reducible with respect to $\mathcal{O}$ for $\ell > 1$. For further details about the decomposition see, for example, Ref. [9].

In our discussion we assume that the infinite volume system has no partial wave mixing, such that orbital angular momentum ℓ is a good quantum number. We also assume that there are no accidental degeneracies in the bound state spectrum, so we can use ℓ as a label for the family of cubic representations split apart at finite volume. Parity invariance remains unbroken by the cubic volume, and we have $P = (-1)^\ell$ just as in the infinite volume case. For clarity, however, we will indicate parity explicitly with $\pm$ superscripts in the following.

With our assumptions, an S-wave state in infinite volume will map onto an A_1^+ state at finite volume. Also a P-wave triplet will map onto the three elements of the T_1^- representation at finite volume. For D-waves, however, the five D-wave states are split into a T_2^+ triplet and an E^+ doublet,

$$D^2 = T_2^+ \oplus E^+\,. \tag{60}$$

In the following we use the notation $|\Gamma, \ell; \alpha\rangle$, $\alpha = 1, \ldots, \dim(\Gamma)$, for the basis vectors of the irreducible cubic representations. We can rewrite the finite volume mass shift in Eq. (38) as

$$\Delta m_B^{(\Gamma,\ell,\alpha)} \equiv \big\langle \Gamma, \ell; \alpha \big| \hat{V} \sum_{|\mathbf{n}|=1} \hat{T}(\mathbf{n}L) \big| \Gamma, \ell; \alpha \big\rangle\,, \tag{61}$$

where $\hat{T}(\mathbf{x})$ is the translation operator by displacement $\mathbf{x}$. We can also calculate the matrix elements of Δm_B in the (ℓ, m) basis. In this case there will be off-diagonal matrix elements connecting (ℓ, m) and (ℓ, m') when m and m' are equivalent modulo 4.

According to Ref. [9], the unitary transformation between the two basis sets for the five D-wave states is

$$\left|T_2^+, 2; 1\right\rangle = -\tfrac{1}{\sqrt{2}} \left(|2,-1\rangle + |2,1\rangle\right) , \tag{62a}$$

$$\left|T_2^+, 2; 2\right\rangle = \tfrac{\mathrm{i}}{\sqrt{2}} \left(|2,-1\rangle - |2,1\rangle\right) , \tag{62b}$$

$$\left|T_2^+, 2; 3\right\rangle = -\tfrac{1}{\sqrt{2}} \left(|2,-2\rangle - |2,2\rangle\right) \tag{62c}$$

and

$$\left|E^+, 2; 1\right\rangle = |2,0\rangle , \tag{63a}$$

$$\left|E^+, 2; 2\right\rangle = \tfrac{1}{\sqrt{2}} \left(|2,-2\rangle + |2,2\rangle\right) . \tag{63b}$$

So, for example, we have

$$\begin{aligned} \Delta m_B^{(T_2^+,2;1)} &= \frac{1}{2}\left(\Delta m_B^{(2,-1,-1)} + 2\Delta m_B^{(2,-1,1)} + \Delta m_B^{(2,1,1)}\right) \\ &= -15|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} \cdot \left(\tfrac{2}{\kappa L} + \tfrac{9}{\kappa^2 L^2} + \tfrac{21}{\kappa^3 L^3} + \tfrac{21}{\kappa^4 L^4}\right) + \mathcal{O}\left(\mathrm{e}^{-\sqrt{2}\kappa L}\right) , \end{aligned} \tag{64}$$

where we have defined

$$\Delta m_B^{(\ell,m_1,m_2)} = (-1)^{\ell+1} \cdot \frac{2\pi\gamma}{\mu} \sum_{|\mathbf{n}|=1} R_\ell^{m_1}\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r\right) \psi^*_{B,(\ell,m_2)}(\mathbf{r}-\mathbf{n}L)\Big|_{\mathbf{r}=0} + \mathcal{O}\left(\mathrm{e}^{-\sqrt{2}\kappa L}\right) \tag{65}$$

as a straightforward generalization of (52).

As expected from cubic symmetry, the mass shift is the same for all three T_2^+ states, and the same for both E^+ states. To summarize our results, we write the mass shift for a state belonging to irreducible representation Γ with angular momentum ℓ as

$$\Delta m_B^{(\ell,\Gamma)} = \alpha\left(\tfrac{1}{\kappa L}\right) \cdot |\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} . + \mathcal{O}\left(\mathrm{e}^{-\sqrt{2}\kappa L}\right) \tag{66}$$

We list the coefficients $\alpha\left(\frac{1}{\kappa L}\right)$ for $\ell = 0, \ldots, 3$ in Table I.

ℓ	Γ	$\alpha(x)$
0	A_1^+	-3
1	T_1^-	$+3$
2	T_2^+	$30x + 135x^2 + 315x^3 + 315x^4$
2	E^+	$-1/2\left(15 + 90x + 405x^2 + 945x^3 + 945x^4\right)$
3	A_2^-	$315x^2 + 2835x^3 + 12285x^4 + 28350x^5 + 28350x^6$
3	T_2^-	$-1/2\left(105x + 945x^2 + 5355x^3 + 19530x^4 + 42525x^5 + 42525x^6\right)$
3	T_1^-	$1/2\left(14 + 105x + 735x^2 + 3465x^3 + 11340x^4 + 23625x^5 + 23625x^6\right)$

TABLE I: Coefficient $\alpha(x)$ in the expression for the finite volume mass shifts for $\ell = 0, \ldots, 3$. Γ indicates the corresponding representation of the cubic group.

B. Sign of the mass shift

The sign of the finite volume mass shift can be understood in terms of the parity of the wave function. In infinite volume the tail of each bound state wave function must vanish at infinity. In the finite volume, however, the bound state wave functions with even parity along a given axis can remain nonzero everywhere. Only the derivative needs to vanish, and the kinetic energy is lowered by broadening the wave function profile. On the other hand, a wave function with odd parity along a given axis must change sign across the boundary. In this case the wave function profile is compressed and the kinetic energy is increased. We have illustrated both cases for a one-dimensional square well potential in Fig. 1.

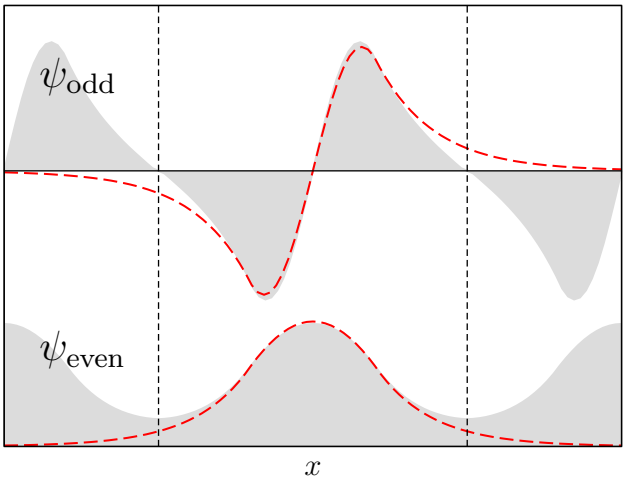

FIG. 1: Wave functions with even (bottom) and odd parity (top) for a one-dimensional square well potential in a box with periodic boundary conditions. The dashed lines give the infinite volume solutions for comparison.

In three dimensions, the situation is slightly more complicated, which can be seen from the fact that for $\ell = 2$ the sign of the mass shift depend on the representation of the cubic group even though the parity is just $(-1)^2 = +1$ for all states. In order to understand this, we consider the basis polynomials for the cubic representations. These basis polynomials are obtained by decomposing the cubic basis vectors in terms of solid harmonics which are homogeneous polynomials in x, y and z. For $\ell = 0, \ldots, 4$ the basis polynomials are also given explicitly in [28].

For a given polynomial $P(x, y, z)$, we define its *leading parity* as

$$\operatorname{lp} P = (-1)^{d_{\max}}, \tag{67}$$

where

$$d_{\max} = \max\{\deg_x P, \deg_y P, \deg_z P\} \tag{68}$$

is the maximum degree of P with respect to any one of the three variables. It is this leading parity that determines the asymptotic behavior of the mass shift as $\kappa L \to \infty$. More precisely, we have

$$\alpha\left(\tfrac{1}{\kappa L}\right) \sim (-1)^{d_{\max}+1} \left(\tfrac{1}{\kappa L}\right)^{\ell - d_{\max}} \quad \text{as} \quad \kappa L \to \infty \tag{69}$$

for the $\alpha\left(\frac{1}{\kappa L}\right)$ in Eq. 66.

It can easily be checked that this relation holds for all results presented in Table I. For $\ell = 2$, for example, we have the basis polynomials

$$P_{2,T_2^+} \sim xy \ , \ yz \ , \ zx \,, \tag{70a}$$

$$P_{2,E^+} \sim x^2 - y^2 \ , \ y^2 - z^2 \,, \tag{70b}$$

and hence $d_{\max} = 1$ for the T_2^+ representation and $d_{\max} = 2$ for the E^+ representation.

C. Trace formula

The expressions for the finite volume mass shift become simpler when we sum over all m for a given ℓ. We can rewrite (52) as

$$\Delta m_B^{(\ell,m)} = (-1)^{\ell+1} \cdot \frac{2\pi\gamma}{\mu} \sum_{|\mathbf{n}|=1} R_\ell^m \left(-\frac{1}{\kappa} \boldsymbol{\nabla}_r \right) \psi^*_{B,(\ell,m)}(\mathbf{r}) \bigg|_{\mathbf{r}=\mathbf{n}L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big) \,. \tag{71}$$

Inserting the asymptotic form of the wave function,

$$\psi^*_{B,(\ell,m)}(\mathbf{r}) \Big|_{\mathbf{r}=\mathbf{n}L} = \left[Y_\ell^m(\theta,\phi) \frac{\mathrm{i}^\ell \gamma \, \hat{h}_\ell^+(\mathrm{i}\kappa r)}{r} \right]^* \Bigg|_{\mathbf{r}=\mathbf{n}L} \,, \tag{72}$$

and using (46) a second time yields

$$\Delta m_B^{(\ell,m)} = (-1)^{\ell+1} \cdot \frac{2\pi|\gamma|^2}{\mu} \sum_{|\mathbf{n}|=1} R_\ell^m \left(-\frac{1}{\kappa} \boldsymbol{\nabla}_r \right) R_\ell^{*m} \left(-\frac{1}{\kappa} \boldsymbol{\nabla}_r \right) \left[\frac{\mathrm{e}^{-\kappa r}}{r} \right] \Bigg|_{\mathbf{r}=\mathbf{n}L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big) \,. \tag{73}$$

Now, from the well-known relation

$$\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi) Y_\ell^{*m}(\theta,\phi) = \frac{2\ell+1}{4\pi} \tag{74}$$

and $R_\ell^m(\mathbf{r}) = r^\ell Y_\ell^m(\theta,\phi)$ we get an analogous expression for the solid harmonics, which then carries over to

$$\sum_{m=-\ell}^{\ell} R_\ell^m \left(-\frac{1}{\kappa} \boldsymbol{\nabla}_r \right) R_\ell^{*m} \left(-\frac{1}{\kappa} \boldsymbol{\nabla}_r \right) f(r) = \frac{1}{\kappa^{2\ell}} \cdot \frac{2\ell+1}{4\pi} \, (\Delta_r)^\ell f(r) \tag{75}$$

for any sufficiently smooth function $f(r)$. Finally, we have

$$(\Delta_r)^\ell \, \frac{\mathrm{e}^{-\kappa r}}{r} = \kappa^{2\ell} \, \frac{\mathrm{e}^{-\kappa r}}{r} \quad (r \neq 0) \,, \tag{76}$$

which follows from Eq. (42). Putting everything together, we arrive at

$$\begin{aligned} \sum_{m=-\ell}^{\ell} \Delta m_B^{(\ell,m)} &= (-1)^{\ell+1} \cdot \frac{2\pi|\gamma|^2}{\mu} \cdot \frac{2\ell+1}{4\pi} \sum_{|\mathbf{n}|=1} \frac{1}{\kappa^{2\ell}} \, (\Delta_r)^\ell \left[\frac{\mathrm{e}^{-\kappa r}}{r} \right] \Bigg|_{\mathbf{r}=\mathbf{n}L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big) \\ &= (-1)^{\ell+1} (2\ell+1) \cdot 3|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big) \,, \end{aligned} \tag{77}$$

where the sum just yields a factor of six. Dividing by $2\ell+1$, we obtain the average mass shift for states with angular momentum ℓ,

$$\Delta m_B^{(\ell)} = (-1)^{\ell+1} \cdot 3|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{78}$$

Apart from the alternating sign, this average shift is independent of ℓ.

Eq. (78) can be verified explicitly for the the results presented in Sec. IV A (*cf.* Table I). For $\ell = 2$, for example, one has to average over the three-dimensional representation T_2^+ and the two-dimensional representation E^+.[3]

V. NUMERICAL TESTS

In order to verify our predictions numerically, we put the Schrödinger equation (19) on a discrete spatial lattice such that the Hamiltonian becomes an ordinary matrix. We then calculate the corresponding energy eigenvalues and eigenvectors.

A. Lattice discretisation

We use a hat symbol to denote dimensionless lattice units. For example, we have

$$\hat{L} = L/a \quad \text{and} \quad \hat{E}_B = E_B \cdot a\,, \tag{79}$$

where a denotes the lattice spacing.

The free lattice Hamiltonian is given by

$$\hat{H}_0 = \sum_{\hat{\mathbf{n}}} \left[\frac{3}{\hat{\mu}}\, a^\dagger(\hat{\mathbf{n}}) a(\hat{\mathbf{n}}) - \frac{1}{2\hat{\mu}} \sum_{l=1,2,3} \big(a^\dagger(\hat{\mathbf{n}}) a(\hat{\mathbf{n}} + \hat{\mathbf{e}}_l) + a^\dagger(\hat{\mathbf{n}}) a(\hat{\mathbf{n}} - \hat{\mathbf{e}}_l) \big) \right] \tag{80}$$

where $a^\dagger(\hat{\mathbf{n}})$ and $a(\hat{\mathbf{n}})$ are creation and annihilation operators for a lattice site $\hat{\mathbf{n}}$ and $\hat{\mathbf{e}}_l$ is a unit vector in the l-direction. The corresponding lattice dispersion relation is

$$\hat{E}(\hat{\mathbf{q}}) = \frac{Q^2(\hat{\mathbf{q}})}{2\hat{\mu}} \tag{81}$$

with the lattice function

$$Q^2(\hat{\mathbf{q}}) = 2 \sum_{l=1,2,3} (1 - \cos \hat{q}_i) = \sum_{l=1,2,3} \hat{q}_l^2 \left[1 + \mathcal{O}(\hat{q}_l^2) \right] \tag{82}$$

and the lattice momenta

$$\hat{\mathbf{q}} = 2\pi \hat{\mathbf{n}} / \hat{L}\,. \tag{83}$$

[3] The mapping from the angular momentum eigenstates to the cubic group states is a unitary transformation.

The binding momentum for a bound state with energy $-\hat{E}_B$ is determined by

$$-\hat{\mu}\hat{E}_B = (1 - \cos(-\mathrm{i}\hat{\kappa})) = (1 - \cosh(\hat{\kappa})) \; . \tag{84}$$

The lattice Green's function for the Hamiltonian (80) is

$$\hat{G}(\hat{\mathbf{n}}, \hat{E}) = \frac{1}{L^3} \sum_{\hat{\mathbf{q}}} \frac{\mathrm{e}^{-\mathrm{i}\hat{\mathbf{q}}\cdot\hat{\mathbf{n}}}}{Q^2(\hat{\mathbf{q}}) + 2\hat{\mu}\hat{E}} \, . \tag{85}$$

We impose periodic boundary conditions by defining the distance $\hat{r}$ to the origin as

$$\hat{r}\,(\hat{\mathbf{n}}) = \sqrt{\sum_{l=1,2,3} \min\left\{\hat{n}_l^2, \left(\hat{L} - \hat{n}_l\right)^2\right\}} \, . \tag{86}$$

B. Methods

We calculate the mass shift using three different methods:

1. As a direct difference in energies, Eq. (20), where we use a very large volume (L_∞) to approximate the infinite volume result.

2. From the overlap formula (38).

3. Using discretized versions of (43) and (53), which we obtain by replacing $\exp(-\kappa r)/r$ with the lattice Green's function. More precisely, we write the asymptotic bound state wave function (17) as

$$\psi_B(\mathbf{r}) = \mathrm{i}^\ell \gamma \, Y_\ell^m(\mathbf{r}/r) \, \hat{h}_\ell^+(i\kappa r) \, \mathrm{e}^{\kappa r} \cdot 4\pi G_\kappa(r) \quad (r > R) \tag{87}$$

and replace the continuum Green's function

$$G_\kappa(\mathbf{r}) = \frac{\mathrm{e}^{-\kappa r}}{4\pi r} \tag{88}$$

with the lattice version

$$\hat{G}_{\hat{\kappa}}(\hat{\mathbf{n}}) \equiv \hat{G}\left(\hat{\mathbf{n}}, \frac{-\hat{\kappa}^2}{2\hat{\mu}}\right) \, . \tag{89}$$

Effectively, this amounts to the replacement

$$\mathrm{e}^{-\hat{\kappa}\hat{L}}/\hat{L} \longrightarrow 4\pi \hat{G}_{\hat{\kappa}}(\hat{L}, 0, 0) \tag{90}$$

in the mass shift formula.

The lattice Green's function is also used to calculate the asymptotic normalization γ from the lattice data. This procedure has the advantage of avoiding large lattice discretization errors.

C. Results

In the following we report physical quantities in units where the reduced mass μ is set to 1.

1. *Gaussian potential*

We first use a Gaussian potential,

$$V_{\text{Gauss}}(r) = -V_0 \, \exp\left(-r^2/(2R^2)\right) \, , \tag{91}$$

with $R = 1$ and $V_0 = 6$. This potential does not have a finite range in a strict mathematical sense, but the range corrections can be entirely neglected in comparison with other errors in our numerical calculation. The smoothness of the Gaussian potential helps to minimize lattice discretization artifacts. In Fig. 2 we show the S- and P-wave mass shifts obtained with the three methods described in Sec. V B above. The results from the three different methods described above agree well for both S- and P-waves. In order to compare the dependence on the box size L with the predicted behavior, we have plotted $\log(L \cdot |\Delta m_B|)$ against L (we use the absolute value of Δm_B since the S-wave mass shift is negative). For both S- and P-waves, the expected linear dependence is clearly visible.

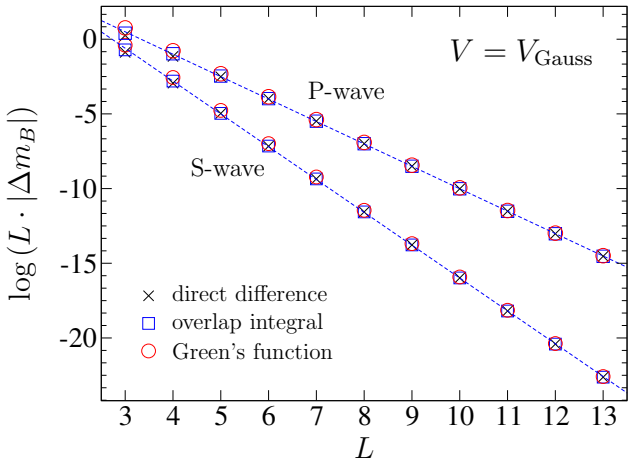

FIG. 2: S-wave and P-wave mass shifts $\log(L \cdot |\Delta m_B|)$ as functions of the box size L (in lattice units) for a Gaussian potential. We show the results obtained from the direct difference Eq. (20) (crosses), evaluation of the overlap integral Eq. (38) (squares), and discretized versions of Eqs. (43), (53) (circles). The dashed lines show linear fits to the overlap integral results.

When we perform a linear fit to the overlap integral data (dashed lines in Fig. 2) we obtain $\kappa = 2.198 \pm 0.005$, $|\gamma| = 11.5 \pm 0.2$ for the S-wave results and $\kappa = 1.501 \pm 0.004$, $|\gamma| = 7.0 \pm 0.1$ for the P-wave results. The values for the asymptotic normalization are in good agreement with the results $|\gamma| \sim 11.5$ (S-wave) and $|\gamma| \sim 7.2$ (P-wave) that are obtained directly from the $L_\infty = 40$ data. Inserting the corresponding energy eigenvalues into the lattice dispersion relation (84), we find $\kappa \sim 2.211$ (S-wave) and $\kappa \sim 1.501$ (P-wave), again in quite good agreement with the fit results. The remaining small discrepancies can be attributed to the mixing with higher partial waves induced by the lattice discretization and the fact that we have not performed a continuum extrapolation to vanishing lattice spacing.

2. *Simple step potential*

For a simple step potential,

$$V_{\text{step}}(r) = -V_0\,\theta(R-r)\,, \tag{92}$$

which we use with $R = 2$ and $V_0 = 3$, the numerical calculation becomes more difficult since the discontinuous shape introduces considerable lattice artifacts. Yet we discuss it here because it has a strict finite range and we find that for a small lattice spacing of $a = 0.2$ the results are satisfactory. In Fig. 3, we show a plot analogous to the one presented for the Gaussian potential. Again, the results from the different methods agree well and the expected linear behavior is clearly visible. Furthermore, the results from the three methods agree well with each other already for smaller L (compared to the results for the Gaussian potential), as expected from the fact that the step potential does not have a tail.

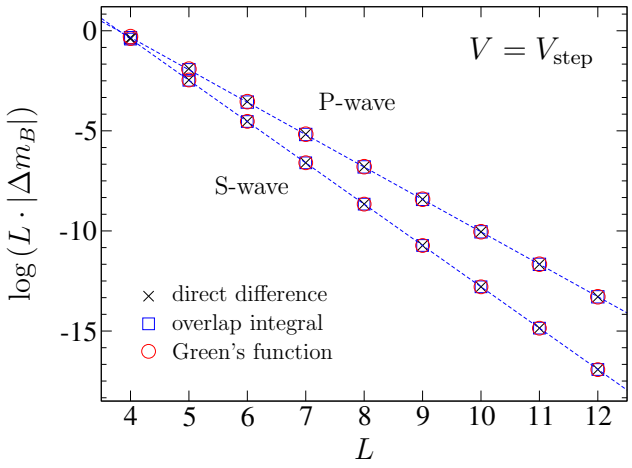

FIG. 3: S-wave and P-wave mass shifts $\log(L \cdot |\Delta m_B|)$ as functions of the box size L (in lattice units) for a simple step potential. The symbols are as in Fig. 2.

From fitting to the overlap integral data (dashed lines in Fig. 3) we obtain $\kappa = 2.0636 \pm 0.0005$, $|\gamma| = 29.17 \pm 0.06$ for the S-wave results and $\kappa = 1.6192 \pm 0.0009$, $|\gamma| = 12.48 \pm 0.05$ for the P-wave results. From the $L_\infty = 40$ data we find $\kappa \sim 2.0666$, $|\gamma| \sim 29.6$ (S-wave) and $\kappa \sim 1.6242$, $|\gamma| \sim 12.8$ (P-wave). Given that we do not have error estimates for the $L_\infty = 40$ results, the overall agreement is quite good.

Finally, we also check our result for the D-wave mass splittings using the step potential with $a = 0.2$. In Fig. 4, we show the mass shift for the D-wave states in both the T_2^+ and the E^+ representation. Due to the polynomial coefficients $\alpha\left(\frac{1}{\kappa L}\right)$ (see Eq. (66) and Table I) one does not expect a linear dependence on L for $\log(L \cdot |\Delta m_B|)$. Hence, we simply plot Δm_B as a function of L directly and do not perform a fit. Nevertheless, we see that (except for very small L, where obviously the condition $L \gg R$ is not satisfied) the agreement between the three methods to calculate Δm_B is very good and hence conclude that our mass shift formula indeed gives the right result also for $\ell = 2$.

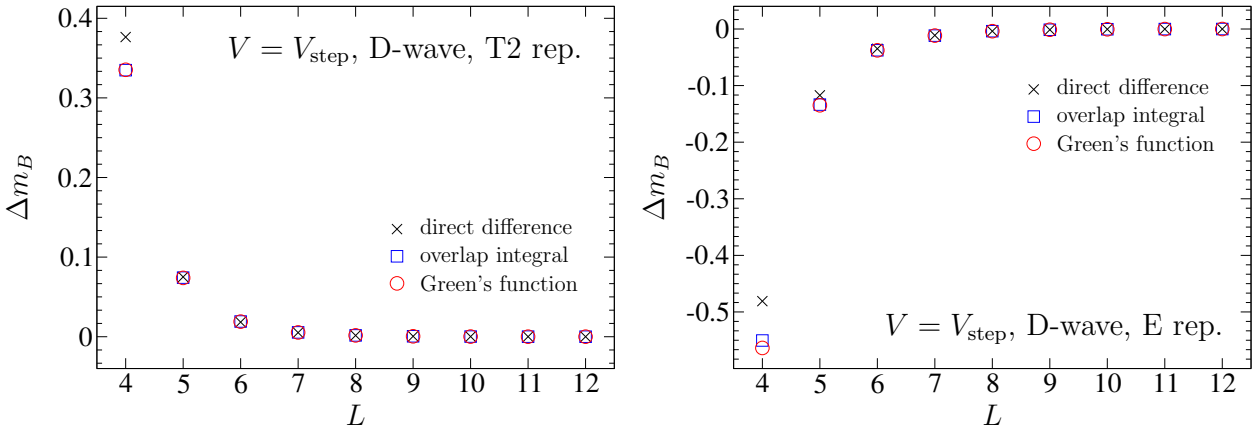

FIG. 4: D-wave, mass shift Δm_B for T_2^+ rep. (left panel) and E^+ rep. (right panel) as a function of the box size L (in lattice units) for a simple step potential. The symbols are as in Fig. 2.

VI. TWO-DIMENSIONAL SYSTEMS

In this section we derive a formula for the finite-volume (or rather finite-area) mass shift of bound states in two-dimensional systems. The results can be used, for example, in lattice simulations of cold atomic systems, which can be prepared experimentally to be effectively two-dimensional [30, 31].

In two dimensions, the Schrödinger equation is

$$-\frac{1}{2\mu}\Delta_r^{\rm 2D}\,\psi_B(\mathbf{r}) + \int \mathrm{d}^2r'\,V(\mathbf{r},\mathbf{r}')\,\psi_B(\mathbf{r}') = -E_B\,\psi_B(\mathbf{r}) \tag{93}$$

with

$$\Delta_r^{\rm 2D}\,\psi_B(\mathbf{r}) = \left[\frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right]\psi_B(\mathbf{r}) \tag{94}$$

in polar coordinates. States are described by a single angular momentum quantum number $m = 0, \pm1, \pm2, \ldots$, and for the wave function we have the separation

$$\psi_B(\mathbf{r}) = u_m(r)Y_m(\theta) \tag{95}$$

with

$$Y_m(\theta) = \frac{\mathrm{e}^{\mathrm{i}m\theta}}{\sqrt{2\pi}}\ . \tag{96}$$

The two linearly independent solutions of the free radial equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{m^2}{r^2} + p^2\right)u_m(r) = 0\,, \tag{97}$$

are just the Bessel and Neumann functions $J_m(pr)$ and $N_m(pr)$. For a bound state, we have $p^2 = -\kappa^2 = -2\mu E_B$, and the wave function has the asymptotic form

$$u_m(r) = \gamma\,K_m(\kappa r) \quad \text{for} \quad r > R\,, \tag{98}$$

where K_m is the modified Bessel function of the second kind. It is related to the Hankel function of the first kind,

$$H_m^{(1)}(z) = J_m(z) + \mathrm{i}N_m(z)\,, \tag{99}$$

via

$$K_m(x) = \frac{\pi}{2}\mathrm{i}^{m+1}H_m^{(1)}(\mathrm{i}x)\,. \tag{100}$$

As in the three-dimensional case, γ is the asymptotic normalization. Inserting (100) into (98) yields a form which is more similar to the three-dimensional expression, Eq. (10). To make the analogy to the calculations in Sec. IV as explicit as possible, we will use the Hankel function in the following intermediate steps and only express the final results in terms of the modified Bessel function.

Nearly all of the three-dimensional calculation carries over and we just replace all exponential terms by Hankel functions. The overlap integral for the mass shift is now

$$\Delta m_B^{(m)} = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^2 r \int \mathrm{d}^2 r'\, \psi_{B,m}^*(\mathbf{r})\, V(\mathbf{r},\mathbf{r}')\, \psi_{B,m}(\mathbf{r}'+\mathbf{n}L) + \mathcal{O}\left(\mathrm{i}H_m^{(1)}\big(\sqrt{2}\kappa L\big)\right)\,. \tag{101}$$

From the asymptotic form of the Hankel function,

$$H_m^{(1)}(z) \sim \sqrt{\frac{2}{\pi z}}\,\mathrm{e}^{\mathrm{i}\left(z-\frac{m}{2}\pi-\frac{\pi}{4}\right)} \quad \text{as} \quad |z|\to\infty\,, \tag{102}$$

it is clear that in principle we still have an exponential behavior. In deriving Eq. (101) we have used this to write

$$\mathcal{O}\left(H_m^{(1)}\big(\mathrm{i}\kappa L\big)^2\right) \sim \mathcal{O}\left(H_m^{(1)}\big(2\mathrm{i}\kappa L\big)\right) \ll \mathcal{O}\left(H_m^{(1)}\big(\sqrt{2}\mathrm{i}\kappa L\big)\right)\,. \tag{103}$$

In the following, we will simply write the correction terms as $\mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)$, as in the three-dimensional case.

The two-dimensional analogue of the relation (46) is

$$Y_m(\theta)H_m^{(1)}(\mathrm{i}\kappa r) = (-\mathrm{i})^m R_m\left(-\frac{1}{\kappa}\boldsymbol{\nabla}^{2\mathrm{D}}\right) H_0^{(1)}(\mathrm{i}\kappa r)\,, \tag{104}$$

where $R_m(r,\theta) = r^m Y_m(\theta)$. This follows from

$$R_m(\boldsymbol{\nabla}^{2\mathrm{D}})f(r) = R_m(\mathbf{r})\left(\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)^m f(r) \tag{105}$$

and

$$\left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^m H_0^{(1)}(z) = (-1)^m\, z^{-m}\, H_m^{(1)}(z) \tag{106}$$

The proof for Eq. (105) can be carried out in the same manner as the three-dimensional proof in Lemma B.1 in [28], where one uses the expansion of $\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{r}}$ (2D vectors) in terms of Bessel functions. As the final ingredient, we have

$$\left[\Delta_r^{2\mathrm{D}} - \kappa^2\right]\frac{\mathrm{i}}{4}H_0^{(1)}(\mathrm{i}\kappa r) = -\delta^{(2)}(\mathbf{r})\,. \tag{107}$$

Using all this in steps completely analogous to those in three dimensions, we get

$$\Delta m_B^{(m)} = (-1)^{m+1} \cdot \frac{\pi\gamma}{\mu} \sum_{|\mathbf{n}|=1} R_m\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r^{2\mathrm{D}}\right) \psi_{B,m}^*(\mathbf{r}-\mathbf{n}L)\Big|_{\mathbf{r}=0} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{108}$$

For $m = 0$ (two-dimensional S-waves), this directly yields

$$\Delta m_B^{(0)} = -2\frac{|\gamma|^2}{\mu} K_0(\kappa L) + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{109}$$

In fact, Eq. (108) can be simplified further. Inserting the asymptotic form for the wave function for $\psi_{B,m}^*$ and using (104) a second time gives

$$\Delta m_B^{(m)} = (-1)^{m+1} \cdot \frac{\pi|\gamma|^2}{\mu} \sum_{|\mathbf{n}|=1} R_m\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r^{2\mathrm{D}}\right) R_m^*\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r^{2\mathrm{D}}\right) \Big[\mathrm{i}\frac{\pi}{2} H_0^{(1)}(\mathrm{i}\kappa r)\Big]\Big|_{\mathbf{r}=\mathbf{n}L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \tag{110}$$

From (96) and $R_m(\mathbf{r}) = r^m Y_m(\theta)$ it is clear that

$$R_m(\theta) R_m^*(\theta) = \frac{(r^2)^m}{2\pi}\,, \tag{111}$$

which then yields

$$R_m\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r^{2\mathrm{D}}\right) R_m^*\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r^{2\mathrm{D}}\right) f(r) = \frac{1}{\kappa^{2m}} \cdot \frac{1}{2\pi} \left(\Delta_r^{2\mathrm{D}}\right)^m f(r) \tag{112}$$

for any sufficiently smooth $f(r)$. This is essentially the same relation that we used to derive the trace formula in the three-dimensional case, only that here we do not have to sum over different m. Together with the two-dimensional analogue of (76),

$$\left(\Delta_r^{2\mathrm{D}}\right)^m H_0^{(1)}(\mathrm{i}\kappa r) = \kappa^{2m} H_0^{(1)}(\mathrm{i}\kappa r) \quad (r \neq 0)\,, \tag{113}$$

we then get

$$\begin{aligned} \Delta m_B^{(m)} &= (-1)^{m+1} \cdot \frac{\gamma|^2}{2\mu} \sum_{|\mathbf{n}|=1} \frac{1}{\kappa^{2m}} \left(\Delta_r^{2\mathrm{D}}\right)^m \Big[\mathrm{i}\frac{\pi}{2} H_0^{(1)}(\mathrm{i}\kappa r)\Big]\Big|_{\mathbf{r}=\mathbf{n}L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big) \\ &= (-1)^{m+1} \cdot \frac{2|\gamma|^2}{\mu} K_0(\kappa L) + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \end{aligned} \tag{114}$$

As we shall see in the following, this is the final result for $m = 0$ and any odd m, whereas for even $m \neq 0$ things become slightly more complicated.

In general, we have to take into account that the finite volume breaks the original planar rotational symmetry of the system down to the symmetry group of a square. We find that states with the same absolute value of m may mix to form good eigenstates in the finite volume. More precisely, we have the symmetric and antisymmetric combinations

$$|m, \pm\rangle = \frac{1}{\sqrt{2}}\big(\,|m\rangle \pm |-m\rangle\,\big) \tag{115}$$

for $m \neq 0$. When we calculate the mass shift for these states (in the same way as described in Sec. IV A), we get mixing terms of the form

$$\Delta m_B^{(m,\text{mixed})} = (-1)^{m+1} \cdot \frac{\pi\gamma}{\mu} \sum_{|\mathbf{n}|=1} R_m\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r^{2\text{D}}\right) \psi^*_{B,-m}(\mathbf{r})\Big|_{\mathbf{r}=\mathbf{n}L} + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \quad (116)$$

Since the condition for the mixing of states is

$$2m \equiv 0 \mod 4\,, \quad (117)$$

they do not play a role for odd m (in fact, they vanish in this case). For even m, however, we have to take them into account and find

$$\Delta m_B^{(m,\pm)} = \frac{1}{2}\left(\Delta m_B^{(m)} \pm 2\Delta m_B^{(m,\text{mixed})} + \Delta m_B^{(-m)}\right) \quad (118)$$

as our final result. As an illustration, we give the explicit results for $|m| = 2$:

$$\Delta m_B^{(2,+)} = -4\frac{|\gamma|^2}{\mu}\left[\left(1 + \tfrac{12}{\kappa^2L^2}\right)K_0(\kappa L) + \left(\tfrac{4}{\kappa L} + \tfrac{24}{\kappa^3L^3}\right)K_1(\kappa L)\right] + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,, \quad (119a)$$

$$\Delta m_B^{(2,-)} = 16\frac{|\gamma|^2}{\mu}\left[\tfrac{3}{\kappa^2L^2}K_0(\kappa L) + \left(\tfrac{1}{\kappa L} + \tfrac{6}{\kappa^3L^3}\right)\right] + \mathcal{O}\big(\mathrm{e}^{-\sqrt{2}\kappa L}\big)\,. \quad (119b)$$

VII. SUMMARY AND OUTLOOK

In this work we have derived explicit formulae for the mass shift of P- and higher-wave bound states in a finite volume and discussed their decomposition into states transforming according to the representations of the cubic group. We have compared our numerical results for $\ell \leq 2$ with numerical calculations of the finite-volume dependence for lattice Gaussian and step potentials and found good agreement with the predictions. For $\ell \geq 2$, the mass shift of a given state (ℓ, m) depends on the angular momentum projection m due to the breaking of rotational symmetry. When we average over all m in a multiplet, however, the absolute value of the mass shift is even independent of ℓ. The mass shift for states in representations of the cubic group, however, is the same for all states. The sign of the mass shift can be understood from the leading parity of the representations. Finally, we have derived corresponding expressions for the finite volume mass shift in two-dimensional systems.

Lattice calculations also provide a method to extract asymptotic normalization coefficients, which are of interest in low-energy astrophysical capture reactions. We have pointed out how the asymptotic normalization and binding momentum of a shallow bound state can be used to extract the effective range from a simulation.

Our work provides a general framework for future lattice studies of molecular states with angular momentum in systems with short-range interactions. Applications to nuclear halo systems and molecular states in atomic and hadronic physics appear promising. An important next step would be to include Coulomb effects into the framework in order to investigate the volume dependence of bound states of charged particles, which are much easier to treat experimentally. In particular, this extension of the formalism is important if one wants to describe proton-halo nuclei. Another interesting direction would be to analyze the volume dependence of resonances along the lines of Refs. [8, 9].

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Appendix A: Shallow binding limit

In this section, we derive the relation between the asymptotic normalization of the bound state wave function and the effective range of the corresponding two-particle scattering process that we have quoted in Sec. II A.

It was already pointed out by Lüscher in [4] that the asymptotic normalization γ of the bound state wave function is related to scattering parameters. More precisely, the analytically-continued elastic scattering amplitude in forward direction has a pole at the bound state energy, and the residue of this pole is proportional to $|\gamma|^2$.

In the limit of shallow bound states, *i.e.*, $\kappa \to 0$, it is possible to make a more direct connection to the effective range in the corresponding scattering channel. The crucial ingredients for this are given in a general investigation of Wigner causality bounds [29]. We express the elastic scattering amplitude $f_\ell(p)$ in terms of the scattering phase shift $\delta_\ell(p)$,

$$f_\ell(p) \propto \frac{p^{2\ell}}{p^{2\ell+1}\left[\cot\delta_\ell(p) - \mathrm{i}\right]}\,, \tag{A1}$$

for which we have the well-known effective range expansion

$$p^{2\ell+1}\cot\delta_\ell(p) = -\frac{1}{a_\ell} + \frac{1}{2}r_\ell\, p^2 + \cdots\,, \tag{A2}$$

where a_ℓ and r_ℓ are the scattering and effective range parameters, respectively. A scattering state is described by a wave function $u_\ell^{(p)}(r)$ that is a solution of the radial Schrödinger equation (3) for positive real center-of-mass momentum $p > 0$. As it is done in [29], we choose the normalization such that outside the range of the potential ($r > R$) we have

$$u_\ell^{(p)}(r) = p^\ell\left[\cot\delta_\ell(p)\,\hat{\jmath}_\ell(pr) + \hat{n}_\ell(pr)\right]\,. \tag{A3}$$

For a bound state, we have $p = \mathrm{i}\kappa$ and $\cot\delta_\ell(p) = \mathrm{i}$. Hence, the wave function is

$$u_\ell^{(\kappa)}(r) = (\mathrm{i}\kappa)^\ell\left[\mathrm{i}\hat{\jmath}_\ell(\mathrm{i}\kappa r) + \hat{n}_\ell(\mathrm{i}\kappa r)\right] = \mathrm{i}^\ell\kappa^\ell\hat{h}_\ell^+(\mathrm{i}\kappa r) \tag{A4}$$

in this case. We immediately see that

$$u_\ell^{(\kappa)}(r) = \frac{\kappa^\ell}{\gamma}u_\ell(r)\,, \tag{A5}$$

where $u_\ell(r)$ is the radial bound state wave function from the previous sections (normalized to 1). Note that the phase convention is chosen such that the wave functions are real. From [29] we have the relation

$$r_\ell = b_\ell(R) - 2\lim_{\kappa\to 0}\int_0^R \mathrm{d}r\left[u_\ell^{(\kappa)}(r)\right]^2 \tag{A6}$$

with

$$\begin{aligned} b_\ell(r) &= -\frac{2\Gamma\left(\ell-\frac{1}{2}\right)\Gamma\left(\ell+\frac{1}{2}\right)}{\pi}\left(\frac{R}{2}\right)^{-2\ell+1} \\ &\qquad - \frac{4}{\ell+\frac{1}{2}}\frac{1}{a_\ell}\left(\frac{R}{2}\right)^{2} + \frac{2\pi}{\Gamma\left(\ell+\frac{3}{2}\right)\Gamma\left(\ell+\frac{5}{2}\right)}\frac{1}{a_\ell^2}\left(\frac{R}{2}\right)^{2\ell+3} \\ &= -\frac{2\Gamma\left(\ell-\frac{1}{2}\right)\Gamma\left(\ell+\frac{1}{2}\right)}{\pi}\left(\frac{R}{2}\right)^{-2\ell+1} + \mathcal{O}(a_\ell^{-1})\,. \end{aligned} \tag{A7}$$

For $\ell = 0$, we get

$$b_0 = 2R + \mathcal{O}(a_\ell^{-1})\,. \tag{A8}$$

Note that $a_\ell^{-1} \to 0$ as $\kappa \to 0$, and since we only consider finite-range potentials, we can in fact write $\mathcal{O}(a_\ell^{-1}) = \mathcal{O}(\kappa)$.

Using the normalization of the wave function we can rewrite (A6) as

$$r_\ell = b_\ell(R) - 2\lim_{\kappa\to 0}\left\{\frac{\kappa^{2\ell}}{\gamma^2} - \int_R^\infty \mathrm{d}r\,\left[u_\ell^{(\kappa)}(r)\right]^2\right\}\,. \tag{A9}$$

The remaining integral can be expressed as

$$\int_R^\infty \mathrm{d}r\,\left[u_\ell^{(\kappa)}(r)\right]^2 = \kappa^{2\ell}\int_R^\infty \mathrm{d}r\,\left[\mathrm{i}^\ell \hat{h}_\ell^+(\mathrm{i}\kappa r)\right]^2\,. \tag{A10}$$

For $\ell = 0$, we get

$$\int_R^\infty \mathrm{d}r\,\left[u_\ell^{(\kappa)}(r)\right]^2 = \frac{\mathrm{e}^{-2\kappa R}}{2\kappa} = \frac{1}{2\kappa} - R + \mathcal{O}(\kappa) \quad \text{as} \quad \kappa \to 0\,. \tag{A11}$$

Together with (A8) this yields

$$r_0 + \frac{2}{\gamma^2} - \frac{1}{\kappa} = \mathcal{O}(\kappa)\,. \tag{A12}$$

Up to the given order this is equivalent to the relation

$$\gamma^2 = \frac{2\kappa}{1-\kappa r_0} \tag{A13}$$

from [26]. For $\ell \geq 1$, the integral is

$$\int_R^\infty \mathrm{d}r\,\left[u_\ell^{(\kappa)}(r)\right]^2 = \frac{\Gamma\left(\ell-\frac{1}{2}\right)\Gamma\left(\ell+\frac{1}{2}\right)}{\pi}\left(\frac{R}{2}\right)^{-2\ell+1} + \mathcal{O}(\kappa) \quad \text{as} \quad \kappa \to 0\,. \tag{A14}$$

We see that the leading term exactly cancels the one in (A7) such that we arrive at

$$r_\ell + \frac{2\kappa^{2\ell}}{\gamma^2} = \mathcal{O}(\kappa)\,. \tag{A15}$$

In all expressions above, the asymptotic normalization of course depends on the binding momentum, *i.e.*, $\gamma = \gamma(\kappa)$, only in general this dependence can not be calculated analytically.

Using the results that we have derived in this paper, it is possible to determine both κ and γ from the volume dependence of a given bound state. If this state is sufficiently shallow, the formulae derived in this chapter can then be used to get an estimate for the effective range of the interaction.

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